A STUDY ON DYNAMICS OF PHYSICO-CHEMICAL PARAMETERS AND CHLOROPHYLL-A IN THE EASTERN ARABIAN SEA, KARNATAKA, INDIA USING IN-SITU AND SATELLITE OBSERVATIONS

SYNOPSIS OF Ph.D. THESIS

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Title of Thesis: A Study on Dynamics of Physico-Chemical Parameters and Chlorophyll-a in the Eastern Arabian Sea, Karnataka, India Using In-Situ and Satellite Observations

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PREFACE:

The ocean plays a fundamental role in regulating the balance of the earth's system. It provides invaluable benefits to humans and marine life. It also serves as a source of economic activity, transportation, providing food, energy production, valuable minerals, commerce and recreation. The ocean plays a fundamental role in climate change, reducing our carbon footprint, acts as a carbon sink, regulates the temperature of the earth, also one of the main sources of oxygen to the life on the planet. In this process, phytoplankton is the key mediator of the biological carbon pump, fixation of atmospheric CO_2 (Basu and Macke, 2018). Coastal waters receive large amounts of nutrients from land and rivers as a result they are found to be rich in phytoplankton biomass. Coastal waters are of great importance as they are potential grounds to provide breeding habitats for many marine species and support a wide range of economic activities, such as tourism, aquaculture, and fishing. The coastal oceans are dynamic and are significantly influenced by upwelling, runoff from land and nutrient flux through rivers and other physical-chemical and ecological processes. These waters are constantly threatened by anthropogenic activities as nearly 65% of the population dwells near the coasts which results in (nutrient) pollution and affects water quality. Human activities are the main current driver of global change that has caused the rise in global temperatures and accelerated nutrient release into coastal areas. Excessive nutrient enrichment (eutrophication) is the root cause of (toxic)

harmful algal blooms that adversely affect marine ecosystems and the people who rely on them. Thus, studying the coastal waters became vital.

Chlorophyll-*a* (chl-*a*) concentration is recognized as an essential water quality parameter and the main representative of phytoplankton biomass (Balali *et al.,* 2013). Indeed, the abundance of phytoplankton biomass potentially indicates the degree of eutrophication which can adversely affect marine ecosystems, biogeochemical cycle by leading to harmful algal blooms, hypoxia and mass mortality of fish (Zheng and DiGiacomo, 2017). Thus, their monitoring is a key component for the effective management of coastal and oceanic resources.

Satellite remote sensing helps to obtain real-time data to study biogeochemical processes, but obtaining accurate ocean color data particularly chl-a in optically complex coastal waters is challenging. Extracting accurate chl-a from ocean color data for Case-1 waters is relatively easier and often yields more accurate results than Case-2 waters (Tilstone *et al.,* 2011, 2013) as chl-a is the major optical constituent that modulates the upwelled light. However accurate chl-a retrievals in many coastal Case-2 waters continue to be hampered by few challenges. One is the retrieval of remote sensing reflectance products within the desired accuracy in the presence of absorbing aerosols (Gordon, 1997). The other is due to the presence of constituents that cause turbidity and is responsible for the failure of the atmospheric correction algorithm, as it violates the black pixel assumption in turbid waters (Siegel *et al.,* 2000). In certain coastal regions, bottom reflectance also adds to the variability in remote sensing reflectance (Menon and Adhikari, 2018). Another major challenge is to retrieve accurate chl-a concentration due to the presence of non-co-varying optically active constituents such as color dissolved organic matter (CDOM) and suspended solids which either absorb or scatter light in wavelengths that are used in the band ratio algorithm for chl-a estimation (Morel *et al.,* 1977; Prieur and Sathyendranath, 1981; Simis *et al.,* 2005; Sathyendranath *et al.,* 1989; Doerffer and Schiller, 2007). Also, it is challenging to use a universal algorithm as most of the algorithms have been developed and validated for the global dataset of *in-situ* measurements obtained for the Case-1 waters and therefore may fail to generate accurate estimates for optically diverse Case-2 waters (Kahru *et al.*, 2014, Jiang *et al.,* 2020). Hence, for more precise estimates in Case-2 waters, these algorithms need to be locally validated and fine-tuned.

Chl-a concentrations and SST are two basic marine physical and biological parameters measured from several satellite sensors which provide insight into biogeochemical processes such as upwelling, convective mixing, nutrients enriched areas, which potentially

support enhanced biological activity. Also, these two are considered important parameters in demarcating potential fishing zones (PFZ) (Solanlki, *et al.*, 2001; Chassot *et al.*, 2010; Nurdin *et al.*, 2013). Other than seasonal cycles, local wind regimes, river inflow, precipitation, currents, stratification, hurricane / tropical cyclone activities, large-scale climatic phenomena such as El Niño Southern Oscillation (ENSO) and Indian Ocean Dipole (IOD) were found to have a significant effect on these parameters (Ashok, *et al,*, 2001; Ummenhofer, *et al.*, 2011; Wada *et al.*, 2012; Moradi, 2020; Thanh *et al.*, 2020). Time-series observation helps to understand the response of these parameters to climatic events. Satellite remote sensing provides time-series data with real-time synoptic global coverage at a regular time interval. In addition to this, machine learning models help in identifying the future trend in the time series (Gupta and Malmgren, 2009; Mahongo and Deo, 2013; Shirvani *et al.*, 2015; Sarkar *et al.*, 2020; Shehhi and Kaya, 2020; Amorim *et al.*, 2021).

SIGNIFICANCE OF THE STUDY:

The marine fisheries are the predominant pelagic resources in Karnataka. Among the three coastal districts of Karnataka, Dakshina Kannada and Udupi districts contributed 38% each, followed by the Uttara Kannada 24% (Kuriakose and Paul, 2017). Southern Karnataka coastal waters are found to continuously being threatened by industrial discharge and domestic effluents discharge as directly flow into the Arabian or through the west-flowing rivers of the region. Some of the previous studies reported deterioration in the water quality of Mangalore coastal waters due to high anthropogenic activities (Avvannavar and Shrihari, 2008; Andrade *et al.*, 2011; Verlecar *et al.*, 2006). Various studies have been conducted on water quality till 2014. Since then a lot of development has taken place in the study area. In this context, this work brings the latest water quality status which is important for the sustainable development and blue economy of Karnataka. Chl-a is one of the important water quality parameters which is amenable to remote sensing but challenging to obtain accurate data from complex coastal waters. This study was conducted using the MODIS Aqua and Terra, SNPP-VIIRS, OC-CCI (merged dataset) and Sentinel-3A (OLCI) to investigate the standard which best represents the chl-a data in the coastal waters of Karnataka. In addition to this, time-series data from the MODIS sensor which is providing data for the longest period since 2002 is used to study spatial and temporal variability of SST & chl-a and the response of these parameters to long-term global oscillations (ENSO and IOD) in coastal and shelf waters off Karnataka, eastern Arabian sea.

OBJECTIVES:

The overall objectives of the present work are to:

1. Study the dynamics and variations of biological and physico-chemical parameters in the coastal waters of southern Karnataka and assessment of water quality.
2. Evaluate the operation of chl-a products from different sensors in the study area using *in-situ* measurements.
3. Study the spatio-temporal variations and abnormality of SST and chl-a time-series data and identify the potential influencing factors in the coastal and shelf waters of Karnataka.
4. Forecast SST and chl-a using Seasonal Autoregressive Moving-Average (SARMA) model.

STRUCTURE OF THE THESIS:

The thesis consists of seven chapters and salient features of each chapter are as described below:

Chapter 1: Introduction

This chapter briefly introduces the role of the ocean in regulating the balance of the Earth's system. It emphasizes the importance of studying the dynamics and status of the coastal waters as it supports a wide range of economic activities, such as tourism, aquaculture, and fishing and is constantly threatened by anthropogenic activities. This chapter also describes the source and dynamics of nutrients as these elements replenish and make waters fertile for the growth of phytoplankton which are the foundations of the food chain. This chapter also summarizes the need for satellite data to study temporal and spatial variations. It also provides insight into the range of sensors that are freely available and challenges to retrieve accurate ocean color data especially chl-a concentration from Case-2 waters. A brief introduction to time series analysis and forecasting is given in this chapter. The physiography of the study area is explained also the significance and objectives of this study are clearly defined.

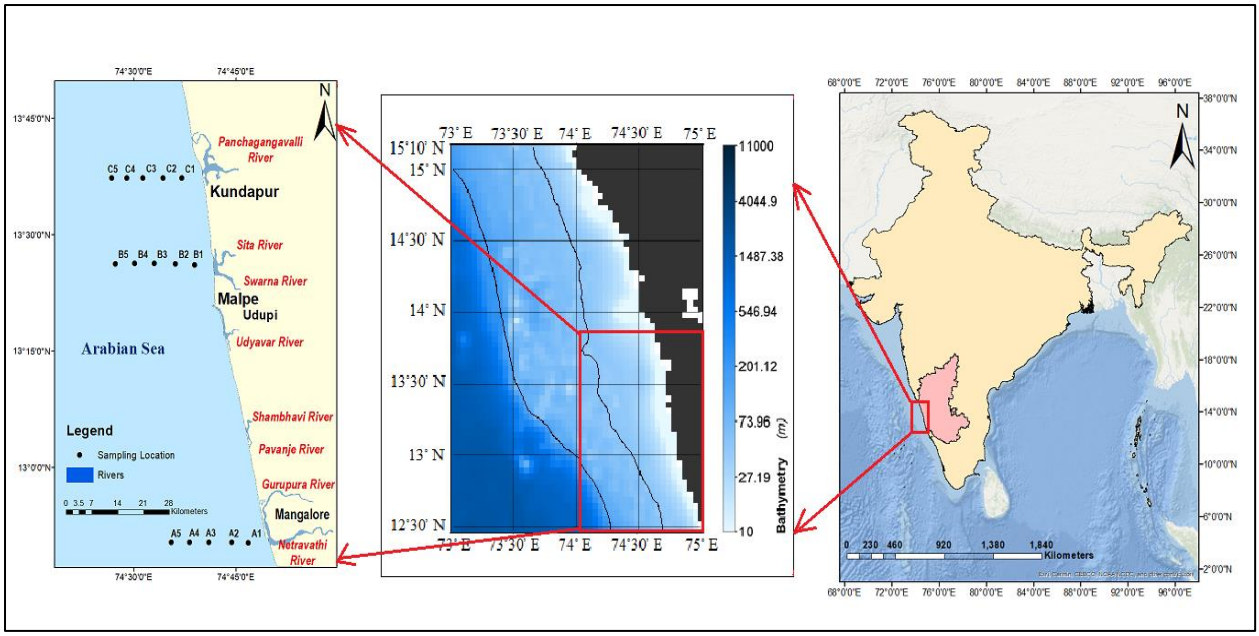


Fig. 1: Map depicts the study area and sampling locations.

Chapter 2: Methods and Techniques

This chapter describes the details of field surveys carried out, the sampling approach / analytical methods used for *in-situ* measurements of various physico-chemical and biological/organic parameters of the water samples such as – water temperature, pH, salinity, phosphate, silicate, nitrite, DO, chl-a, TSM, etc. This chapter also includes the descriptive statistics and multivariate statistical methodologies such as Principle Component Analysis (PCA), correlation analysis, cluster analysis which were incorporated to unmask the hidden patterns of distribution and interdependency between biological and physico-chemical parameters during different seasons and to assess the water quality of the eastern Arabian Sea from Mangalore to Kundapur. These statistical analyses were carried out in IBM SPSS and XLSTAT.

In addition to these, brief details of satellite data (chl-a images) acquisition and processing from different sensors to obtain high spatial resolution images are explained. As the standard products of VIIRS-SNPP, MODIS Aqua and Terra are available in 4 km and 9 km, image processing was carried out in SeaDAS (Ubuntu OS) to generate one km images and SENTINEL OLCI images were processed in SNAP application to generate high (300 m and one km) resolution data. These data were validated against *in-situ* measurements and uncertainties were quantified using statistical metrics to check for the best product which closely represents the field data in the study area.

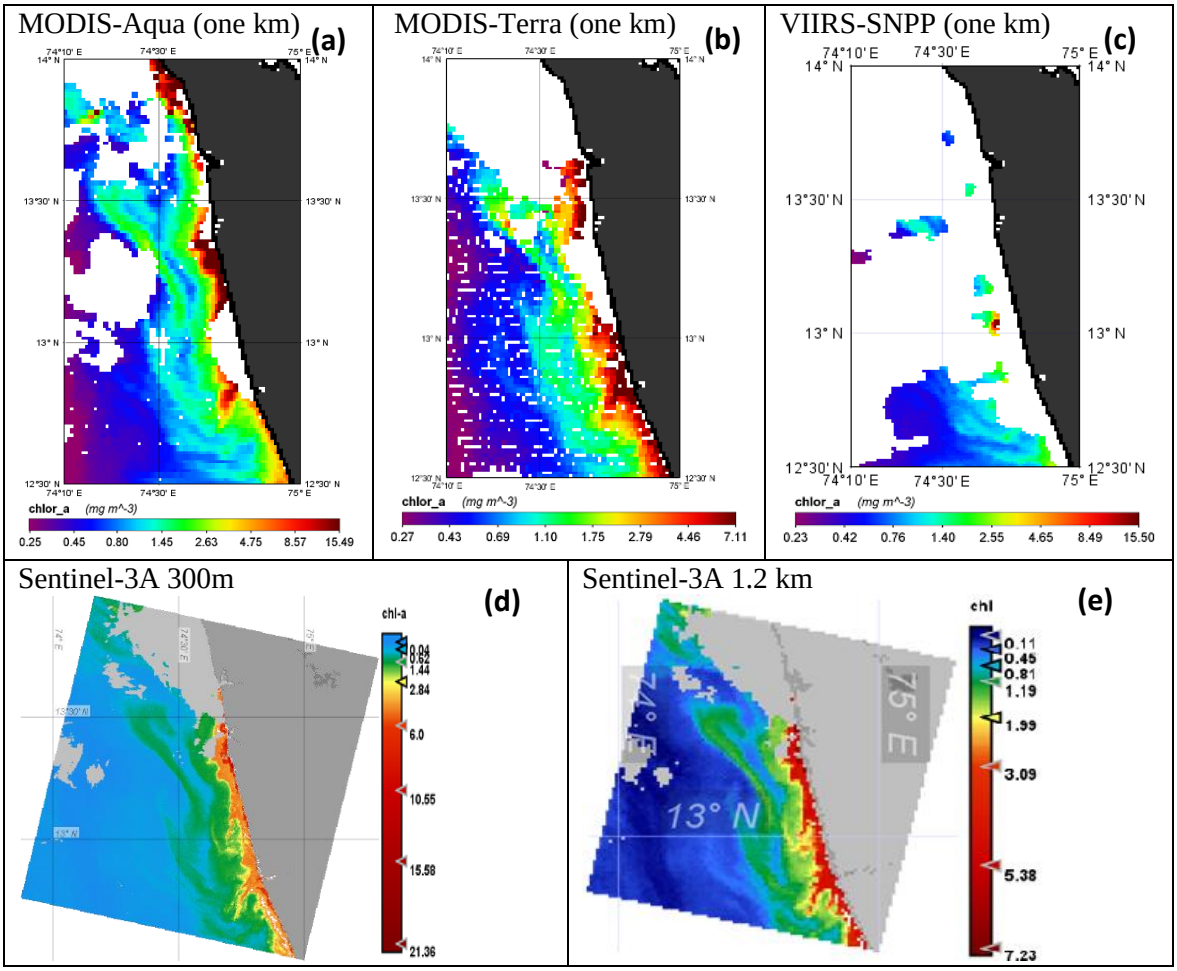
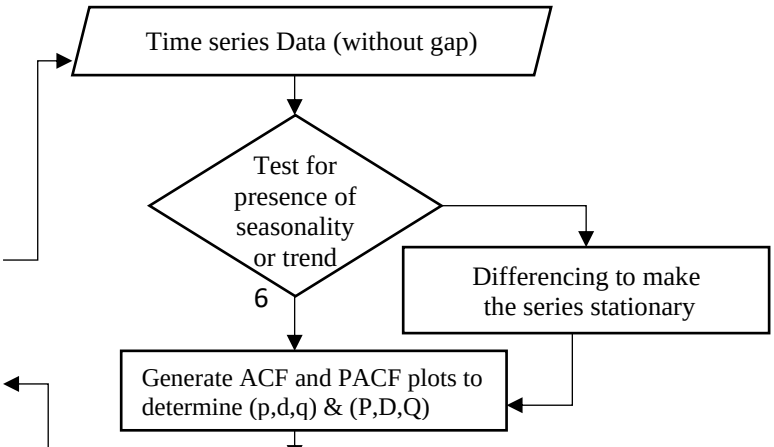


Fig. 2: (a) - (e) are MODIS-Aqua, MODIS-Terra, VIIRS-SNPP, Sentinel-3A derived full resolution (mg/m^3) and reduced resolution images of chl-a of 20 December of 2016.

Further, time-series data of MODIS Aqua, GPM_3IMERGM were also used to study the temporal variations of chl-a, SST and precipitation. Yearly anomalies of these parameters were calculated for coastal (0-50 m depth) and shelf region waters (50-200 m) to understand long-term variation and to associate their response to large scales climatic phenomena like ENSO events (El Niño and La Niña) and IOD. Monthly and spatial anomalies were studied using monthly climatology. Also, an attempt has been made to forecast SST and chl-a variations over the offshore waters off Karnataka for the 24 months using the mathematical / machine learning model such as Seasonal Autoregressive Moving-Average (SARMA) model.


Time series Data (without gap)
Test for presence of seasonality or trend
Differencing to make the series stationary
Generate ACF and PACF plots to determine (p,d,q) & (P,D,Q)

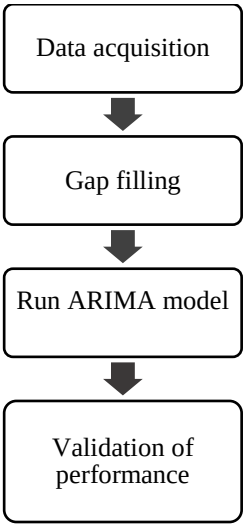


Fig. 3: Flowchart showing the steps followed to generate the forecast of SST and chl-a.

Chapter 3: Spatio-temporal variation of bio-physicochemical parameters and assessment of coastal water quality using multivariate statistical analysis

The current study concerns examining the spatiotemporal and vertical dynamics of physico-chemical and bio/organic parameters collected during three different seasons – North-East monsoon (NEM), Summer Inter-monsoon (SIM) and Winter seasons from 2016 to 2018. The findings reveal Mangalore and Malpe coastal waters are more influenced by anthropogenic activity than Kundapur coastal waters. Dissolved oxygen-depleted waters were encountered in the study area during the study period.

In addition, the collected parameters were subjected to multivariate statistical analyses such as PCA, Correlation Analysis, which were found to be the effective method to interpret the relationship in the complex data set to assess the water quality of the study area.

By using the Pearson Correlation method, correlation matrices were generated and interrelationships between the parameters were studied which altogether is responsible for the change in entire marine biota during different seasons. Also, the potential source of nutrients that indirectly represents the pollution state was identified. R mode cluster analysis was performed and dendrograms were constructed to identify the association between biological and physico-chemical parameters during three different (NEM, SIM and Winter) seasons.

PCA analysis was carried out separately for different seasons. An attempt was made to explain the cause of changes in the system and based on a few significant parameters depending on the loading of the parameters on the components. Also, PCA observation plots were found to be useful in identifying the presence of zonation or stratification in the water column.

The effect of post-depression (cyclone) induced precipitation and river runoff on physicochemical parameters during NE monsoons was discussed. As both NEM 2016 and 2017 witnessed cyclone Vardah and Ockhi respectively well mixing of the vertical column was noticed in the PCA observation plots. PCA observation plots found to be useful for discerning patterns within the data set.

Chapter 4: Validation of the operational Chl-a product from global ocean color sensors in the coastal waters, south-eastern Arabian Sea

In this chapter, the standard chl-a product from MODIS Aqua and Terra, SNPP-VIIRS, OC-CCI (merged dataset) and Sentinel-3A (OLCI) were compared with the in-situ chl-a to evaluate the performance of different operational chl-a products /algorithms, at different spatial resolutions in the coastal waters of southern Karnataka, Arabian Sea. The uncertainties in these products are poorly quantified for many regional seas and coastal waters. To validate and quantify the uncertainty of satellite retrieved chl-a with respect to field measurements**,** statistical metric**s** such as Log_RMSE, Log_bias, RMSE, MAPD and MRPD were used.

MODIS Aqua and Terra-derived chl-a of 4 km resolution tend to overestimate in the nearshore as shown by a high mean relative percentage difference (MRPD) of 77.09%, and a low coefficient of determination (R^2) of 0.35. A significant improvement was seen for MODIS one km resolution chl-a product (R^2 = 0.64, bias = 22.30%) and Mean Absolute Percentage Deviation (MAPD) = 47.08%. Validation of SNPP-VIIRS derived chl-a of 4 km with *in-situ* measurements showed moderate correlation (R^2 = 0.54, MAPD = 49.21%), whereas one km SNPP-VIIRS showed substantially better result than 4 km with majority of data points aggregated along the 1:1 line (R^2 = 0.86, MAPD = 43.66%, MRPD = 20.97%). Chlorophyll-a product at original resolution (750 m) showed less error than 4 km and one km resolution (MAPD = 39.18%, R^2 = 0.75, MRPD = 10.875%). In contrast, OC-CCI underestimated field measured chl-a concentrations as indicated by MRPD (-36.72%), with moderate R^2 = 0.58. All 4 km data showed poor results than higher spatial resolution data.

The Sentinel-3A OLCI FR (C2RCC OLCI processed) Chl-a-NN product at 300 m, was found to closely represent the field measured data and satellite-derived chl-a data were most accurate in the coastal waters of the study area. Sentinel-3A OLCI 300 m full-resolution (FR) derived chl-a, showed R^2 = 0.80, MAPD = 33.07%, and MRPD = 23.89%, whereas Sentinel-3A reduced-resolution (RR-1.2 km) exhibited slight overestimation (MRPD = 28.43%, MAPD = 39.88%, R^2 = 0.78) than Sentinel-3A(FR). An uncertainty of 33% indicated that the neural network approach takes care of the other optical constituents present in the coastal waters. While for coarse-resolution (1.2 km) product of Sentinel-3A uncertainty increased to 39.9%. indicating the importance of spatial resolution.

Comparison of operational chl-a product from OC-CCI, MODIS, SNPP-VIIRS, and Sentinel-3A OLCI illustrated that Sentinel-3A OLCI performed best in coastal waters of Karnataka. The spatial resolution and the retrieval algorithm of the satellite imagery were found to be the important factors determining the accuracy of chl-a in coastal waters. Analysis of the operational chl-a product reveals the importance of finer spatial scales as optical constituents are not distributed uniformly and patchiness is an inherent property of the coastal waters.

As few images of Aqua and Terra were available due to cloud cover both data sets were combined for comparison with *in-situ*. Therefore, to understand and quantify the performance of MODIS Terra and Aqua (one km) individually, an inter-sensor comparison was carried out. Both sensors were also compared with SNPP-VIIRS as SNPP-VIIRS (one km) product had higher accuracy with less errors. For comparing these sensors, the same number of pixels (N = 437) common over the region has been considered and subjected to a similar statistical analysis.

Comparison of chl-a from MODIS Terra with Aqua in the coastal region (bathymetry up to 50 m) shows that Terra overestimated Aqua chl-*a* data by 6.65% (MRPD), and 0.017 in terms of Log_bias. The corresponding MAPD was 19.80%, and RMSE = 0.37 mg/m^3 (Log_RMSE = 0.1). A similar comparison between MODIS Aqua and SNPP-VIIRS shows the observed bias to be 15.93% (Log_bias = 0.06) implying that MODIS-Aqua has overestimated the SNPP-VIIRS with MAPD = 17.3% and slightly lower errors than Terra v/s Aqua (RMSE = 0.28 mg/m^3, Log_RMSE = 0.083). In the case of MODIS Terra with SNPP-VIIRS overestimation was higher than MODIS Aqua (bias = 22.95%, Log_bias = 0.077). The MAPD (27.64%) was quite high compared to MODIS Aqua. Also, error estimators show

slightly high values (RMSE = 0.496 mg/m^3, Log_RMSE = 0.129). Hence, the result reveals that the performance of MODIS Aqua is more comparable to SNPP-VIIRS than MODIS-Terra.

Chapter 5: Time series analysis of SST and Chl-a in the coastal and shelf waters of south-eastern Arabian Sea using satellite data

The aim of this study is to investigate the spatial and inter-annual variations/ dynamics of SST and chl-a in coastal (0-50 m depth) and shelf region (50-200 m) of the south-eastern Arabian Sea along the Karnataka Coast and to identify the associated factors responsible for the anomaly. In this study, we have used 18 years (between 2003 and 2020) of monthly SST and chl-a concentrations derived from ocean color products of the MODIS Aqua sensor. As MODIS Aqua provides the data for the long duration from 2002 to the present and has comparatively better accuracy than MODIS-Terra it was used for the time series analysis. In addition, 18 years of rainfall data from Integrated Multi-satellite Retrievals for GPM (Global Precipitation Measurement) (IMERG) - GPM_3IMERGM v06 were used.

The merged 18-year (2003-2020) time series of SST shows a long-term increasing trend comparatively higher in coastal waters than shelf waters. While chl-a showed a decreasing trend in coastal waters over time.

The results revealed a high anomaly of SST and chl-a in certain years which coincide with the ENSO and IOD years. SST and chl-a of both coastal waters and shelf waters off Karnataka appeared to be significantly influenced by the monsoon and also responsive to positive IOD negative IOD, El Niño and La Niña events according to the intensities of their modes. Also, the combined effect of ENSO and IOD events is studied.

Chapter 6: Forecast of SST and Chl-a using SARIMA, south-eastern Arabian Sea, Karnataka, India.

In this chapter an attempt has been made to forecast SST and chl-a variations using the Seasonal Autoregressive Moving-Average (SARMA) model over the offshore waters off Karnataka, south-eastern Arabian Sea. This study focuses on the modelling of SST and chl-a time series data to predict their future values at two years lead over the offshore waters of Karnataka which covers both coastal and shelf regions of the Arabian Sea. For this purpose,

we have used 18 years of SST and chl-a data derived from MODIS Aqua and evaluated the accuracy of the model using statistical metrics over the study region.

The time profile plots of the SST and chl-a time series data were generated to check for the presence of seasonality and trend and we observed that there is seasonality in the data. To confirm the same Rank Sum test and Mann Kendall Test were carried out. From the result, it was concluded that there is seasonal variation in the data and the absence of a trend component. Thus, seasonal differencing was carried out to make the series stationary. Hence the value of the seasonal difference is D=1 and due to the absence of trend component, trend difference order d=0. From ACF and PACF plots of SST and chl-a data (p, d, q) (P, D, Q) values were taken i.e. p=2, q=3, d=0, P=3, D=1, Q=2 and p=1, q=2, d=0, P=3, D=1, Q=2 respectively and the seasonal period is taken S=12 as it is monthly data. Out of several combinations of (p, d, q) (P, D, Q) values better model was chosen based on the Lower Akaike Information Criterion (AIC) and higher Ljung box p-value and Box pierce p-value. SARIMA [1,0,1] $[1,1,2]_{12}$ for SST and SARIMA [1,0,0] $[3,1,1]_{12}$ for chl-a had minimum AIC value and maximum p-value compared to all other models. Hence, these models were used forecasting SST and chl-a respectively. This model is used to forecast SST and chl-a for the next 24 months.

Performance of the SARIMA model predicted values against satellite-derived values were assessed using a set of cross-validation methods. In the literature Root Mean Square Error (RMSE), Mean Relative Percentage Error (MAPE) and Mean Absolute Relative Percentage Error (MRPE) and Goodness of fit (using the coefficient of determination (R^2) slope and intercept) are widely adopted as performance indicators.

The SARIMA model best fits SST data which is clear from the high value of the coefficient of determination (R^2 =0.87) which is near to perfect fit value 1 and from the linear regression line obtained slope (0.876) was close to 1:1 line. Also, very less errors – RMSE (0.351), MAPE (0.905%) and negligible overestimation by the model revealed by MRPE =0.047%. Hence SARIMA modelled SST was found to show good agreement with the original / satellite extracted SST data with an accuracy of about 99%.

The errors for modelled chl-a are found to be comparatively higher than modelled SST (RMSE = 0.671). The coefficient of regression R^2 (0.53) for the SARIMA model generated chl-a and satellite-derived data is found to be less and match-up points are found to be scattered

around the trend line with a slope value of 0.50. This shows the model can capture only about 50% of the variance of the original chl-a data set, which is also clear from the MAPE value of 51.266. The SARIMA model for chl-a is found to largely underestimate the satellite-derived chl-a which is clear from the MRPE value (-29.38%).

The cross-validation results exhibit that this method is more effective in modelling SST than chl-a time series and predicting future values, as the error for the modelled chl-a is higher than SST. The anomaly maps were generated from climatology to check for the spikes in the time series. Frequencies of high chl-a anomaly observed during monsoon and post-monsoon seasons are more than the inter-monsoon seasons. Moreover, from the time series anomaly, it was found that the magnitude of the chl-a anomaly is considerably higher than SST. The poor performance of SARIMA in estimating chl-a concentration is due to the complexity of the (Case-2) coastal waters and the high level of spikes caused due to the bloom conditions during monsoon or post-monsoon seasons which is clear from the chl-a anomaly plot.

Chapter 7: Summary and Conclusions

This chapter summarises all findings from chapters 2 to 6 and highlights the important conclusion of the present research work. The most significant highlight of the thesis is the present coastal water quality of southern Karnataka and pinpoint of the best satellite product which can be used for studies on phytoplankton in this region which in turn promote the blue economy of Karnataka. Time series analysis of SST and chl-a data help to identify how the long-term events such as ENSO and IOD affect their variation and forecasting techniques to predict their future trend. This chapter will also describe the future perspectives of present research and recommendations for future works.

Research Paper published

- Harshada, D., Raman, M., and Jayappa, K. S. (2021). Evaluation of the operational Chlorophyll-a product from global ocean colour sensors in the coastal waters, south-eastern Arabian Sea. *The Egyptian Journal of Remote Sensing and Space Science*. https://doi.org/10.1016/j.ejrs.2021.09.005

Manuscript communicated

- Harshada, D., Raman, M., Deepak P. R. and Jayappa, K. S. "Multivariate Analyses of Coastal Water Quality Parameters off Southern Karnataka, south-eastern Arabian Sea".

Conference full papers:

- "Forecast of Sea Surface Temperature and Chlorophyll-a using ARIMA, South-Eastern Arabian Sea, Karnataka, India" paper presented on International Virtual Conference on Innovative Trends in Hydrological and Environmental Systems (ITHES-2021) held at National Institute of Technology Warangal. ISBN No: yet to get (in press).

- "A study on variability and inter-relationship of Coloured Dissolved Organic Matter and salinity in shallow marine waters off Udupi-Dakshina Kannada districts" Deepak, P. R., Harshada, Jayappa, K. S. (UGC sponsored two days National Seminar on Earth Resources Conservation and Management held during 01-02 July 2019 at Kuvempu University, Shivamogga).

Papers presented

- "Variability of chlorophyll-a and its response to physico-chemical parameters in the eastern Arabian sea". Harshada, Deepak P. R., Jayappa K. S., and Mini Raman (Poster presentation at National Conference on Reaching the Unreached Through Science and Technology held during Sept.,8-9,2017 at Mangalore University in association with The Indian Science Congress Association).

- "Effect of spatial resolution on the operational chlorophyll-a product in the coastal waters of southern Karnataka, India". Harshada D. and K. S. Jayappa (Oral presentation on International online Conference WAVELENGTH 2021 held during 17-18 March 2021 at University of Stirling, United Kingdom in association with Remote Sensing & Photogrammetry Society (RSPSoc.)).

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